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ON OPTIMAL CHEBYSHEV-TYPE QUADRATURES

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ABSTRACT

A well-known result of S. N. Bernstein states that a Chebyshev quadrature formula of the form

$$\int_{-1}^{1} f(x)dx = \frac{2}{n} \sum_{k=1}^{n} f(t_{k}) + R_{n}(f), \quad t_{k} \text{ real },$$

can have algebraic degree of exactness p=n only if $1 \le n \le 7$ or n=9. The nodes t_k are necessarily symmetric with respect to the origin, so that in fact p=2[n/2]+1. If symmetry of the nodes is imposed, it is known from work of Gautschi and Yanagiwara and others that next-to-highest algebraic degree p=2[n/2]-1, beyond the classical cases above, can be attained only when n=8, 10, 11, and 13. For these values of n, "optimal" formulas have been obtained which minimize $|R_n(\mathbf{x}^{p+1})|$ among all symmetric Chebyshev quadratures of degree p=2[n/2]-1. We show here that these same formulas in fact minimize $|R_n(\mathbf{x}^i)|$ for each $i \ge p+1$.

AMS(MOS) Subject Classification - 65D30, 41A55

Key Words - Chebyshev-type quadrature formulas; constrained optimization;

Sturm sequences; power sums of zeros of polynomials.

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ON OPTIMAL CHEBYSHEV-TYPE QUADRATURES

Walter Gautschi and Giovanni Monegato

1. <u>Introduction</u>. We consider symmetric Chebyshev-type quadrature formulas of "next-to-highest" algebraic degree of exactness, i.e., equally weighted quadrature formulas of the form

(1.1)
$$\int_{-1}^{1} f(x)dx = \frac{2}{n} \sum_{k=1}^{n} f(t_k) + R_n(f) ,$$

subject to the following constraints,

(1.2)
$$\begin{cases} \text{all } t_k \text{ are real, } t_1 \ge t_2 \ge \dots \ge t_n \text{ ,} \\ t_{n+1-k} + t_k = 0, \quad k = 1, 2, \dots, n \text{ (symmetry),} \\ R_n(f) = 0 \text{ for every polynomial } f \text{ of degree } p = 2[n/2]-1. \end{cases}$$

If $1 \le n \le 7$, or n = 9, the classical Chebyshev quadratures satisfy all these conditions, the last one in the strengthened form with p = 2[n/2] + 1. Other Chebyshev-type formulas, satisfying (1.2), exist only for n = 8, 10, 11, and 13. This is shown in [6] and [1], where formulas are derived that are "optimal" in the sense of minimizing

(1.3)
$$\rho(t_1, t_2, \dots, t_n) = |R_n(x^{p+1})|, \quad p = 2[n/2] - 1,$$

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subject to (1.2). Each of these formulas has one pair of symmetric double nodes, or one double node at the origin, which (regretfully) means loss of the equal coefficient property. We will show here that these same formulas are in fact optimal in the much wider sense of minimizing

(1.4)
$$\rho_{i}(t_{1}, t_{2}, ..., t_{n}) = |R_{n}(x^{i})|$$
 for each $i \geq p + 1$,

subject to (1.2). (For odd integers i, the statement is trivially true, since ρ_i = 0 by virtue of symmetry.) In particular, they are minimum norm quadratures in the Hardy space H_2 of functions f(z) analytic in |z| < r, r > 1, and square-integrable on |z| = r, since these quadratures minimize $\sum_{j=p+1}^{\infty} r^{-2j} [R_n(x^j)]^2 \text{ (see, e.g., [2])}.$

As a preliminary step toward these results, we first show that for each n=8, 10, 11, 13, the set of all Chebyshev-type quadrature formulas (1.1), satisfying (1.2), forms a one-parameter family, with parameter α in some finite closed interval $\lambda_n \leq \alpha \leq \mu_n$. By using symbolic Sturm sequences, we are able to identify λ_n and μ_n as roots of certain algebraic equations. The quadrature formulas corresponding to $\lambda_n < \alpha < \mu_n$ all have n distinct (simple) nodes in the interval (-1,1), while those corresponding to $\alpha = \lambda_n$ or $\alpha = \mu_n$ have a pair of symmetric double nodes, or a double node at the origin. The main result then follows from a (possibly new) monotonicity property satisfied by the power sums of the zeros of a polynomial. In particular, it transpires that the optimal formulas [in the general sense of minimizing (1.4)] always occur at $\alpha = \lambda_n$. They are necessarily identical with the optimal formulas found in [6] and [1].

2. One-parameter families of Chebyshev-type quadratures. We associate with (l. l) the polynomial

$$\xi(x) = \prod_{k=1}^{n} (x-t_k) = x^n + a_1 x^{n-1} + \dots + a_n$$
.

From Newton's identities it follows that the (real ordered) nodes $\ t_k$ will satisfy (1.2) if and only if

(2.1)
$$\xi(x) = \begin{cases} x^n + a_2 x^{n-2} + \dots + a_{n-2} x^2 + \alpha & (n \text{ even}), \\ \\ x^n + a_2 x^{n-2} + \dots + a_{n-3} x^3 + \alpha x & (n \text{ odd}), \end{cases}$$

where α is some real parameter and the coefficients a_2, a_4, \dots, a_{p-1} (p = 2[n/2]-1) are given uniquely by

$$\begin{cases} s_2 + 2a_2 = 0, \\ s_4 + a_2s_2 + 4a_4 = 0, \\ \dots \\ s_{p-1} + a_2s_{p-3} + \dots + a_{p-3}s_2 + (p-1)a_{p-1} = 0, \end{cases}$$

where

$$s_{2j} = \frac{n}{2} \int_{-1}^{1} t^{2j} dt = \frac{n}{2j+1}, \quad j = 1, 2, ..., (p-1)/2.$$

It remains to determine the conditions on α under which the polynomial ξ in (2.1) has only real zeros. Letting

$$\xi(x) = \begin{cases} \xi^*(x^2) & (n \text{ even}), \\ x\xi^*(x^2) & (n \text{ odd}), \end{cases}$$

we are seeking the conditions on α under which the polynomial

(2.3)
$$\xi^*(x) = x^{\nu} + a_2 x^{\nu-1} + \dots + a_{2\nu-2} x + \alpha, \quad \nu = \lfloor n/2 \rfloor,$$

has only nonnegative zeros. While the problem could easily be discussed in geometric terms, we prefer to take an algebraic approach via Sturm sequences. Among other things, this allows us to identify the limits on the parameter α as roots of certain algebraic equations with integer coefficients.

We recall that the Sturm sequence of a polynomial p_0 of degree ν is the result of applying Euclid's algorithm to p_0 and $p_1 = p_0$, where p_0 is the derivative of p_0 . Thus,

(2.4)
$$\begin{cases} p_0 = q_1 p_1 - p_2, \\ p_1 = q_2 p_2 - p_3, \\ \dots \\ p_{\tau-2} = q_{\tau-1} p_{\tau-1} - p_{\tau}, \\ p_{\tau-1} = q_{\tau} p_{\tau}, \end{cases}$$

where $\tau \leq \nu$, and each p_{κ} , $2 \leq \kappa \leq \tau$, is the negative remainder of the division of $p_{\kappa-2}$ by $p_{\kappa-1}$. Sturm's theorem (see, e.g., [3, p. 448]) then asserts that for any a < b, if $p_0(a) p_0(b) \neq 0$, the number of distinct zeros of p_0 in [a,b] is equal to v(a) - v(b), where v(x), for fixed x, is the number of sign changes in the numerical sequence $p_0(x)$, $p_1(x)$, ..., $p_{\tau}(x)$. Moreover, if x_0 is a (real or complex) zero of p_0 , then its multiplicity is m if and only if x_0 is a zero of the terminal polynomial

 p_T of multiplicity m-1. In particular, all zeros of p_0 in [a,b] are simple if and only if p_T has no zeros in [a,b].

In wishing to apply this to the polynomial $p_0 = \xi^*$ in (2.3), one has to be prepared to operate on polynomials whose coefficients depend rationally on the parameter α . This is best done with the help of symbolic formula manipulation systems. We indeed generated the Sturm sequences symbolically, using the MACSYMA system available to one of us at Stanford University, and repeating the computations with the SAC-1 system on the UNIVAC 1110 computer at the University of Wisconsin. The results of both computations were identical, and are summarized below.

Writing

$$p_{\kappa}(x) = c_{\kappa\kappa} x^{\nu-\kappa} + c_{\kappa, \kappa+1} x^{\nu-\kappa-1} + \dots + c_{\kappa\nu}, \quad \kappa = 0, 1, \dots, \nu,$$

the coefficients $c_{\kappa\lambda}$, $\kappa\leq\lambda$, are polynomials or rational functions of α , with rational coefficients, the degrees of which are as indicated in the schedules below. Zero degree always represents a non-vanishing (rational) constant; slashes separate numerator degree from denominator degree in case of rational functions. In all rational functions on the diagonal, the denominator polynomial is the square of the numerator polynomial in the rational

$n=8 \ (\nu=4)$	$n=10, 11 \ (\nu=5)$		1	n=]	13	(v=	6)	
0 0 0 0 1	0 0 0 0 0 1	0	0	0	0	0	0	1
0 0 0 0	0 0 0 0 0		0	0	0	0	0	0
0 0 1	0 0 0 1			0	0	0	0	1
1 1	0 1 1				0	0	1	1
3/2	2 2					1	1	1
	4/4						3/2	2 3/2
								7/6

function preceding it on the diagonal. The numerator polynomials in the terminal entries are irreducible over the field of rationals, except in the case of n = 13, where the numerator polynomial of c_{66} factors into the square of a linear polynomial and a polynomial of degree five.

According to Sturm's theorem, the polynomial ξ^* has ν distinct positive zeros (necessarily all simple) if and only if $v(0) = \nu$ and $v(\infty) = 0$, that is, if and only if

(2.5)
$$c_{\kappa\kappa} > 0 \text{ and } (-1)^{\nu-\kappa} c_{\kappa\nu} > 0 \text{ for } \kappa = 0, 1, 2, ..., \nu$$
.

By examining the explicit form of these (polynomial) inequalities for the four values of n under study, one finds that (2.5) is equivalent to

$$\lambda_{n} < \alpha < \mu_{n} ,$$

where λ_n and μ_n are either zero, or equal to one of the zeros $\alpha_1^{(n)} < \alpha_2^{(n)} < \alpha_3^{(n)} < \dots \text{ of } c_{\nu\nu}(\alpha), \text{ as indicated in Table 2.1. Numerical}$

n	λ_{n}	μ_n
8	0	α(8) 2
10	$\alpha_2^{(10)}$	0
11	$\alpha_2^{(11)}$	$\alpha_3^{(11)}$
13	$\alpha_2^{(13)}$	$\alpha_3^{(13)}$

Table 2.1. Parameter intervals for symmetric Chebyshev-type formulas of next-to-highest degree

values of λ_n , μ_n , and the numerator polynomial $c_{\nu\nu}^N$ of $c_{\nu\nu}$ in exact integer form (of which $\alpha_2^{(n)}$, $\alpha_3^{(n)}$ are zeros) are shown below.

By verifying that $v(1)=v(\infty)=0$ for α in the interval (2.6), one finds that all ν zeros of ξ^* are in fact strictly between 0 and 1.

n = 8

 $C_{44}^{N}(\alpha) = 107661642834375\alpha^{3} - 1739295676125\alpha^{2} + 1639058085\alpha + 1698929$

 $\lambda_8 = 0$

 $\mu_8 = 1.696315226301022019273508 \times 10^{-3}$

n = 10

 $c_{55}^{N}(\alpha) = 103836101679541153125\alpha^{4} - 699972937051972500\alpha^{3}$ $- 118379410645986\alpha^{2} + 59483935980\alpha + 10026277$

 $\lambda_{10} = -1.705026344541702458795446 \times 10^{-4}$

 $\mu_{10} = 0$

n = 11

 $-32517908999837432625626726400000\alpha^{2}$

 $-17819369567349884423809920000\alpha - 2271280061895695934118607$

 $\lambda_{11} = -7.231729443377509440273227 \times 10^{-4}$

 $\mu_{11} = -1.843814365405786592111158 \times 10^{-4}$

[†] For n = 13, only the factor (of degree 5) of $c_{\nu\nu}^{N}$ is shown which is relevant.

 $\lambda_{13} = 1.024260940958103474931671 \times 10^{-4}$ $\mu_{13} = 1.325979284585333715590553 \times 10^{-4}$

The Sturm sequence terminates prematurely [i.e., $\tau < \nu$ in (2.4)] if and only if α is a zero of one of the diagonal entries $c_{\kappa\kappa}$. We examined the Sturm sequence in each one of these cases and found, as expected, that ξ^* has the desired number of nonnegative zeros precisely when α is a nonzero endpoint of the parameter intervals in Table 2.1. In each case, ξ^* has one double zero and ν - 2 simple zeros in the open interval (0,1).

The remaining endpoint $\alpha=0$ in the cases n=8 and n=10 can be handled by forming the Sturm sequences at $x=\epsilon>0$ sufficiently small, and at x=1. One finds $\nu-1$ simple zeros of ξ^* in (0,1), which together with the zero at x=0 again yields the desired number of zeros in [0,1).

We may summarize our findings in terms of the polynomial ξ in (2.1) as follows: If n = 8, 10, 11, or 13, the polynomial ξ has n real

(symmetric) zeros, counting multiplicities, exactly if α is in the interval $\lambda_n \leq \alpha \leq \mu_n$. If α is an interior point of that interval, all zeros of ξ are in fact simple and contained in the open interval (-1,1). If α is one of the endpoints of $[\lambda_n, \mu_n]$, then ξ has a pair of (symmetric) double zeros in (-1,1), if $\alpha \neq 0$, and a double zero at the origin, if $\alpha \approx 0$, all other zeros being simple and located in (-1,1).

The intervals $[\lambda_n, \mu_n]$ found here are in agreement with the (less accurate) intervals given in [4, Table I] for n=8, 10, and 11. Our results for n=8 and n=10 contradict a theorem of Pecka [5], which indeed is false because of computational errors in the proof.

3. Optimal Chebyshev-type formulas. In each one-parameter family of Chebyshev-type quadratures, obtained in Section 2, we now wish to single out one that minimizes the objective function ρ_i in (1.4). We may assume i=2j, with $j\geq \nu$, where $\nu=\lceil n/2\rceil$. Letting $t_\kappa^*(\alpha)$ denote the zeros of ξ^* , and

$$s_{j}^{*}(\alpha) = \sum_{\kappa=1}^{\nu} [t_{\kappa}^{*}(\alpha)]^{j}, \quad j = 0, 1, 2, ...,$$

their power sums, and assuming $\lambda_n \leq \alpha \leq \mu_n,$ the objective function is easily found to be

(3.1)
$$\rho_{2j}^{*}(\alpha) = \frac{4}{n} |s_{j}^{*}(\alpha) - \frac{n}{2(2j+1)}|, \quad j \geq \nu.$$

We thus wish to minimize $\rho_{2j}^*(\alpha)$ on the interval $\lambda_n \leq \alpha \leq \mu_n$. The lemmas which follow will lead us to the solution of this problem.

Lemma 3.1. Suppose the algebraic equation

$$g(x) := x^{m} + c_{1}x^{m-1} + ... + c_{m-1}x + c_{m} = 0$$
,

with real coefficients c_{μ} , has m distinct nonnegative roots $x_k = x_k(c_l)$, c_2, \ldots, c_m , $k = l, 2, \ldots, m$. Let s_j denote their j-th power sum,

$$s_j(c_1, c_2, ..., c_m) = \sum_{k=1}^{m} [x_k(c_1, c_2, ..., c_m)]^j, j = 0, 1, 2, ...$$

Then

(3.2)
$$\frac{\partial s_{j}}{\partial c_{\mu}} < 0 \quad \underline{if} \quad j \ge \mu, \quad \underline{and} \quad \frac{\partial s_{j}}{\partial c_{\mu}} = 0 \quad \underline{if} \quad j < \mu .$$

<u>Proof.</u> Since, by Newton's identities, s_j depends only on c_1, c_2, \ldots, c_j , the second half of (3.2) is self-evident. It suffices, therefore, to consider $j \ge \mu$, $1 \le \mu \le m$.

Differentiating the identity $g(x_k(c_1, c_2, \dots, c_m)) \equiv 0$ with respect to c_μ , one finds

$$\frac{\partial x_k}{\partial c_{\mu}} = -\frac{x_k^{m-\mu}}{g'(x_k)} = -\frac{x_k^{m-\mu}}{\prod\limits_{\ell \neq k} (x_k - x_{\ell})},$$

hence

(3.3)
$$\frac{\partial s_{j}}{\partial c_{\mu}} = j \sum_{k=1}^{m} x_{k}^{j-1} \frac{\partial x_{k}}{\partial c_{\mu}} = -j \sum_{k=1}^{m} \frac{x_{k}^{m-\mu+j-1}}{\prod_{\ell \neq k} (x_{k}^{-x} - x_{\ell}^{\ell})}.$$

The sum on the far right is precisely the (m-l)-st divided difference $[x_1,x_2,\ldots,x_m] f \text{ of the function } f(x)=x^{m-\mu+j-l} \text{. Since}$

 $[x_1, x_2, \ldots, x_m] f = f^{(m-1)}(\overline{x})/(m-1)! = (\frac{m-\mu+j-1}{m-1}) \overline{x}^{j-\mu}$, where \overline{x} is in the open interval spanned by x_1, x_2, \ldots, x_m , and since all $x_k \ge 0$, it follows that $\overline{x} > 0$, and the sum in question is positive. This proves the lemma.

We remark that the proof of Lemma 3.1 also yields $\frac{\partial s_j}{\partial c_\mu} \ge 0$ if j < 0, if we assume all $x_k > 0$, but we will not need this fact in what follows.

<u>Lemma 3.2.</u> <u>If</u> n = 8, 10, 11, <u>or</u> 13, <u>we have</u>

(3.4)
$$s_{j}^{*}(\lambda_{n}) < \frac{n}{2(2j+1)} \text{ for } j \geq \nu$$
.

<u>Proof.</u> Since the quadrature formula (1.1) has polynomial degree of exactness $p = 2\nu - 1$, it is certainly exact for $f(x) = x^{2\nu - 2}$, which yields

(3.5)
$$s_{\nu-1}^* = \frac{n}{2(2\nu-1)}.$$

For any $j \ge \nu$, we have

$$s_{j}^{*}(\alpha) = \sum_{\kappa=1}^{\nu} \left[t_{\kappa}^{*}(\alpha)\right]^{j-\nu+1} \left[t_{\kappa}^{*}(\alpha)\right]^{\nu-1} < \left[t_{1}^{*}(\alpha)\right]^{j-\nu+1} s_{\nu-1}^{*}, \quad \lambda_{n} \leq \alpha \leq \mu_{n},$$

where $t_1^*(\alpha)$ is the largest among the roots $t_\kappa^*(\alpha)$. The lemma will hold for any value of j for which

$$[t_1^*(\lambda_n)]^{j-\nu+1} s_{\nu-1}^* < \frac{n}{2(2j+1)}$$
.

By virtue of (3.5), this is equivalent to

(3.6)
$$t_1^*(\lambda_n) < (\frac{2\nu-1}{2j+1})^{\frac{1}{j-\nu+1}}$$

An elementary computation shows that the right-hand expression in (3.6) is an increasing function of j for $j \ge \nu$. By consulting the numerical values of $t_1(\lambda_n)$ in [1], and noting that $t_1^*(\lambda_n) = \left[t_1(\lambda_n)\right]^2$, it is possible to verify the validity of (3.6) for $j = \nu + 2$ when n = 8, for $j = \nu + 3$ when n = 10, for $j = \nu + 4$ when n = 11, and for $j = \nu + 5$ when n = 13. The inequality therefore holds for these and all larger values of j. For the few remaining values of j, one can verify (3.4) directly, from the data available in [1]. This completes the proof of Lemma 3.2.

The problem of minimizing $p_{2j}^*(\alpha)$ in (3.1) is now easily solved.

Theorem 3.1. If n = 8, 10, 11, or 13, then for each $j \ge \nu$,

$$(3.7) \qquad \qquad \rho_{2j}^*(\lambda_n) < \rho_{2j}^*(\alpha) \quad \underline{\text{for}} \quad \lambda_n < \alpha \le \mu_n .$$

<u>Proof.</u> Applying Lemma 3.1 to the polynomial ξ^* in (2.3), the zeros of which are $t_{\kappa}^*(\alpha)$, we find that each $s_j^*(\alpha)$, $j \geq \nu$, is strictly decreasing on $\lambda_n < \alpha < \mu_n$, hence

(3.8)
$$s_{j}^{*}(\alpha) < s_{j}^{*}(\lambda_{n}) \text{ for } \lambda_{n} < \alpha \leq \mu_{n}.$$

Combining (3.8) with Lemma 3.2 gives

$$s_j^*(\alpha) < \frac{n}{2(2j+1)}, \quad \lambda_n < \alpha \le \mu_n$$
,

for each $j \ge \nu$. Since $s_j^*(\alpha)$ decreases on $\lambda_n < \alpha < \mu_n$, it follows that $\rho_{2j}^*(\alpha)$ is an increasing function of α , hence (3.7).

Corollary. Let $\{w_j\}$ be any sequence of weights $w_j \ge 0$, with $w_j > 0$ for some $j \ge \nu$, satisfying

(3.9)
$$\sum_{j=\nu}^{\infty} j^{-2} w_{j} < \infty ,$$

and let

(3.10)
$$\rho^*(\alpha) = \sum_{j=\nu}^{\infty} w_j [\rho_{2j}^*(\alpha)]^2, \quad \lambda_n \leq \alpha \leq \mu_n.$$

Then

(3.11)
$$\rho^*(\lambda_n) < \rho^*(\boldsymbol{\alpha}) \quad \underline{\text{for}} \quad \lambda_n < \alpha \le \mu_n .$$

Proof. Since $s_j^*(\alpha) < \nu[t_1^*(\alpha)]^j$, where $t_1^*(\alpha)$ is the largest among the roots $t_\kappa^*(\alpha)$, and since $t_1^*(\alpha) < 1$ for $\lambda_n \le \alpha \le \mu_n$, the sequence $s_j^*(\alpha)$ tends to zero at least geometrically, and consequently $\rho_{2j}^*(\alpha) \sim j^{-1}$ as $j \to \infty$. The infinite series in (3.10), therefore, converges by virtue of (3.9), and (3.11) is an immediate consequence of (3.7).

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Gautschi and Yanagiwara and others that next-to-highest algebraic degree p=2[n/2]-1, beyond the classical cases above, can be attained only when n=8, 10, 11, and 13. For these values of n, "optimal" formulas have been obtained which minimize $|R_n(x^{p+1})|$ among all symmetric Chebyshev quadratures of degree p=2[n/2]-1. We show here that these same formulas in fact minimize $|R_n(x^i)|$ for each $i \ge p+1$.